One-dimensional Van Hove polaritons

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We study the light-matter coupling of microcavity photon and interband transition in a one-dimensional (1D) nanowire. Due to the Van Hove singularity in the density of states resulting in resonant character of the absorption line the achievement of strong coupling becomes possible even without formation of a bound state of an electron and a hole. The calculated absorption in the system and corresponding energy spectrum reveal anti-crossing behavior characteristic to the formation of polariton modes. Contrary to the case of conventional exciton polaritons, formation of 1D Van Hove polaritons will not be restricted to low temperatures and can be realized in any system with a singularity in the density of states.

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I. INTRODUCTION

Light-matter coupling is an area of research emerging at the boundary between condensed matter physics and optics which has both fundamental and applied dimensions. The possibility to reach the regime of strong coupling, for which confined cavity photons and matter excitations are strongly mixed, is of particular interest.[1] In this situation a new type of elementary excitations, known as polaritons, appear in the system. Having a hybrid nature, they combine the properties of both light and matter. Several geometries were proposed for the realization of the regime of strong coupling.

The interaction of a cavity photon mode with a two-level system which mimics optical transitions in an individual atom or single quantum dot (QD) is the origin of cavity quantum electrodynamics (cavity QED).[2,3] One should note that the achievement of strong coupling in such a system is a non-trivial task due to a rather small light-matter interaction constant. However, recent advances in nanotechnology have led to the possibility of creating high-finesse optical cavities and have resulted in the observation of Rabi doublet and Mollow triplet in the emission spectrum of individual QDs.[4–6] Moreover, the strong coupling of a single photon to a superconducting qubit, which has a two-level structure as well, was demonstrated in a radiowave superconducting cavity.[7]

To increase light-matter coupling, quantum wells (QWs) can be used instead of individual QDs. In this case, coupling occurs between a 2D QW exciton, associated with a sharp absorption peak slightly below the bandgap energy, and a photonic mode of a planar cavity tuned in resonance with it. Observed for the first time two decades ago,[8] exciton-polariton physics is now experiencing a boom connected to to the possible realization of polariton lasing with an extremely low threshold,[9] and the achievement of Bose-Einstein condensate (BEC),[10] and superfluid states[11] for temperatures much higher than for atomic systems[12,13] and cold excitons in solids.[14] This is a consequence of the small effective mass of polaritons which allows a pronounced manifestation of quantum collective phenomena for a critical temperature around 20 K in CdTe structures[10] and even at room temperatures in wide band gap materials with large exciton binding energy and strong light-matter interaction (GaN, ZnO).[15,16] Additionally, polaritons were proposed as basic ingredients for spinoptronic devices[17] and all-optical logical elements and integrated circuits.[18,19]

Another system where strong light-matter coupling was experimentally achieved is intersubband transitions in quantum wells (QWs). It was shown by D. Dini and co-workers[20] that the absorption of intersubband resonance placed into a cavity reveals the characteristic anti-crossing behavior. The attractive peculiarity of such a system in comparison to those based on conventional interband exciton-polaritons is a non-vanishing ratio of Rabi frequency to transition energy, which enables an exploration of the ultra-strong coupling regime.[21] In addition, different to interband transitions in a 2D system, strong electron-hole interactions and the formation of excitons are not necessary for obtaining the strong coupling regime,[22] although they play a certain role in structures with highly doped QWs, where the formation of intersubband plasmon-polaritons[24,25] and Fermi edge polaritons[26] can be observed.

For any experimental geometry, the main condition which must be satisfied to drive the system into strong coupling is the presence of a narrow resonance in its photoabsorption spectrum. Mathematically, this condition reads

$$g = \hbar\Omega_R \gg \gamma_{cav} - \gamma_{ex}, \tag{1}$$

where g denotes the light-matter coupling strength, Ω_R is the corresponding Rabi frequency (light-matter interaction constant), γ_{cav} is the damping constant of the cavity mode and γ_{ex} is the width of the absorption resonance.[1,23] In 2D interband absorption this condition requires strong exciton-hole attraction resulting in the

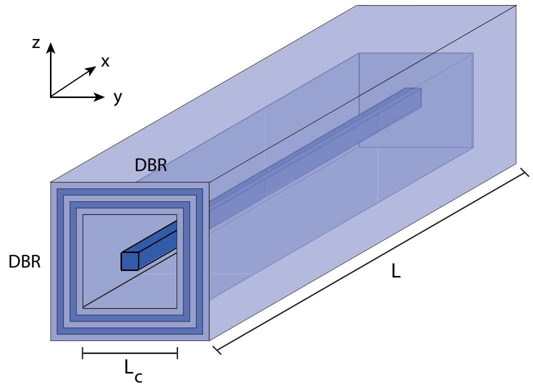

FIG. 1. (Color online) A sketch of the system. A semiconductor microcavity is formed with two pairs of Bragg mirrors (DBR) with cavity width in z and y direction being L_c. The length of 1D semiconductor wire is L.

formation of an exciton. However, in the 1D case this is not strictly speaking necessary, since the behavior of the density of states $\rho(E)$ in 2D and 1D is qualitatively different. In the former case, the density of states is constant, while in the latter it diverges around the points E_0 at which the energy as a function of the momentum k reaches its minimum,

$$\rho(E) \sim \frac{1}{\sqrt{E-E_0}}. \tag{2}$$

This peculiarity, known as a Van Hove singularity, makes optical properties of 1D nanostructures different from bulk and 2D cases and leads to the resonant character of photoabsorption even without any excitonic effects.

In this article we analyze the possibility of the realization of the strong coupling regime between a cavity photon and interband transition of one-dimensional (1D) nanowire driven by the presence of the Van Hove singularity in the 1D density of states. We demonstrate that the spectrum of the elementary excitation reveals anti-crossing behavior characteristic to the formation of polaritonic modes for realistic cavity quality factors.

II. MODEL

We consider a system consisting of a 1D semiconductor wire embedded into an optical microcavity (see sketch in Fig. 1), which is tuned into resonance with a direct interband transition.

To calculate an optical response of the coupled wire-resonator system, we use a many-body approach based on Green's functions. Information about the dispersion of elementary excitations in the coupled quantum wire-cavity system can be extracted from the poles of the Green's function of the cavity photon interacting with interband transition $D(q,\omega)$. The absorption spectrum can be determined from the polarization operator $\Pi(q,\omega)$. The formalism we are going to use is analogous to the one developed in Ref. [25] for intersubband transitions.

We start with a calculation of the polarization operator, accounting for the possibility of multiple re-emissions and re-absorptions of a cavity photon by interband transition in the quantum wire. These corresponding processes can be represented graphically as an infinite set of diagrams, as shown in Fig. 2(a), which can be reduced to the Dyson equation shown in Fig. 2(b). Its solution reads

$$\Pi(k,\omega) = \frac{\Pi_0(k,\omega)}{1-g^2 D_0(k,\omega)\Pi_0(k,\omega)}, \tag{3}$$

where g is the light-matter coupling constant, D_0 is a propagator of the cavity photon, given as[25]

$$D_0(k,\omega) = \frac{2\omega_{cav}(k)}{\hbar\omega^2 - \hbar\omega_{cav}^2(k) - 2i\gamma\omega_{cav}(k)}, \tag{4}$$

with the dispersion of the cavity photon being

$$\hbar\omega_{cav}(k) \approx \frac{\hbar^2 k^2}{2m_{ph}} + E_g + \delta, \tag{5}$$

where m_{ph} is an effective mass of the cavity photon defined by the geometry of the cavity, and δ is the detuning between the cavity mode and bandgap E_g. $\gamma = h/\tau_{ph}$ represents the damping of the cavity mode appearing due to the imperfectness of the cavity, where τ_{ph} is the cavity photon lifetime.

In Eq. (3) Π_0 is a polarization operator of the wire in absence of the cavity. Strictly speaking, its calculation requires a full account of the many-body interactions in the system and thus represents a formidable problem. In the current work, however, we are interested in effects of the Van Hove singularity only, and thus the approximation of non-interacting particles will be applied in the further discussion. In this case, $\Pi_0(q,\omega)$ is represented by a "bubble" diagram and can be calculated as

$$i\Pi_0(q,\omega) = -\int \frac{dk}{2\pi/L}\frac{d\nu}{2\pi/\hbar}[iG_e(k+q,\nu+\omega)iG_h(k,\nu) + iG_h(k+q,\nu+\omega)iG_e(k,\nu)]. \tag{6}$$

Here $G_e(q,\omega)$ and $G_h(q,\omega)$ are the Green's functions of an electron in the conductance band and a hole in the valence band, respectively,

$$G_e(q,\omega) = \frac{1}{\hbar\omega - E_g - \hbar^2 q^2/2m_e + i\epsilon}, \tag{7}$$

$$G_h(q,\omega) = \frac{1}{\hbar\omega + \hbar^2 q^2/2m_h - i\epsilon}, \tag{8}$$

where m_e and m_h are the effective electron and hole masses (both taken to be positive) and E_g is the energy gap of the semiconductor wire. An analytical integration of Eq. (6) leads to an explicit expression for the bare

polarization operator Π_0:

$$\Pi_0(q,\omega)=\frac{L\sqrt{2\mu}}{\hbar}\left(\frac{f_1(q,\omega)}{\sqrt{\hbar\omega+E_g+\hbar^2q^2/M-i\epsilon}}+\right.$$

$$\left.+\frac{if_2(q,\omega)}{\sqrt{\hbar\omega-Eg-\hbar^2q^2/M+i\epsilon}}\right), \quad (9)$$

where μ denotes the reduced mass, $\mu^{-1}=m_e^{-1}+m_h^{-1}$, and $M=m_e+m_h$. The functions $f_1(q,\omega)$ and $f_2(q,\omega)$ are given by

$$f_1(q,\omega)=\frac{1}{\pi}\left[\tan^{-1}\left(\frac{\pi/a+\beta_e q}{\sqrt{2\mu(\hbar\omega+E_g+\hbar^2q^2/M-i\epsilon)}}\right)\right.$$
$$\left.+\tan^{-1}\left(\frac{\pi/a-\beta_e q}{\sqrt{2\mu(\hbar\omega+E_g+\hbar^2q^2/M-i\epsilon)}}\right)\right], \quad (10)$$

$$f_2(q,\omega)=-\frac{i}{\pi}\left[\tanh^{-1}\left(\frac{\pi/a+\beta_h q}{\sqrt{2\mu(\hbar\omega-E_g-\hbar^2q^2/M+i\epsilon)}}\right)\right.$$
$$\left.+\tanh^{-1}\left(\frac{\pi/a-\beta_h q}{\sqrt{2\mu(\hbar\omega-E_g-\hbar^2q^2/M+i\epsilon)}}\right)\right], \quad (11)$$

where L is a length of the wire, and we have introduced the notations $\beta_e=m_e/M$ and $\beta_h=m_h/M$. Parameter a defines the cut-off of the integration $\pm\pi/a$ and is proportional to the size of elementary cell of the material of the wire. For small momentum q the functions are close to unity in all frequency range.

The light-matter coupling constant g can be calculated as[27]

$$g=|d_{cv}|\sqrt{\frac{\hbar\omega_{cav}}{2\epsilon\epsilon_0 V}}\approx\sqrt{\frac{\hbar^2e^2}{\epsilon\epsilon_0\mu L_c^2 L}}, \quad (12)$$

where $\hbar\omega_{cav}$ denotes the energy of the photonic mode, ϵ and $V=L_c^2L$ are the dielectric permittivity and volume of the cavity, respectively, and the cavity length parameters L_c and L are shown in the geometry sketch (Fig. 1).

The polarization operator Π_0 has both real and imaginary parts, and the latter is related to the absorption coefficient of the electron-hole interband excitation:[27]

$$\alpha(\omega)=\frac{4\pi\omega}{n_b c}\chi''(\omega)=\frac{4\pi\omega}{n_b c}\frac{|d_{cv}|^2}{V_{QW}}\Im\Pi_0(q,\omega), \quad (13)$$

where $\chi''(\omega)=\frac{|d_{cv}|^2}{V_{QW}}\Im\Pi_0(q,\omega)$ is the imaginary part of the optical susceptibility, $V_{QW}=LA$ is the volume of the quantum wire, A is the wire's cross-section and n_b is a background refractive index. If the cavity is absent and one assumes a vertical transition, the absorption of 1D nanowire reads[27]

$$\alpha_0(\omega)=\frac{4\pi\sqrt{2\mu}|d_{cv}|^2}{n_b\hbar cA}\omega\frac{1}{\sqrt{\hbar\omega-E_g}}\Theta(\hbar\omega-E_g). \quad (14)$$

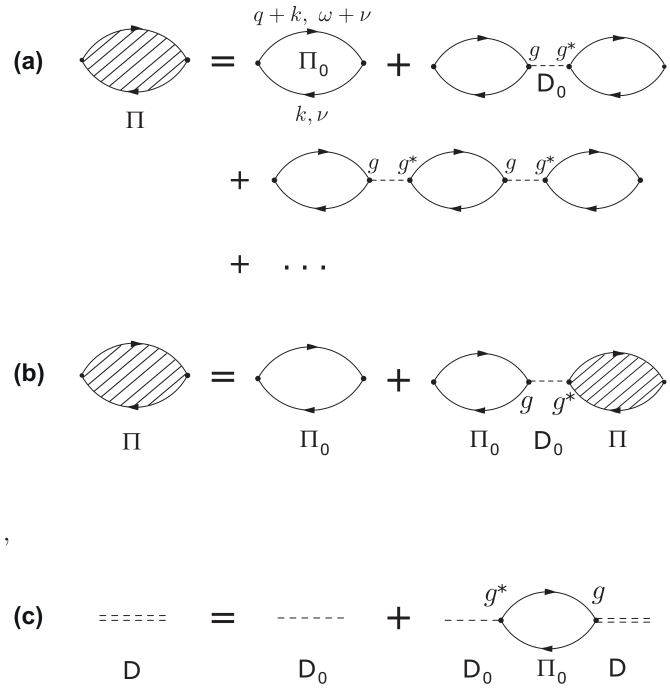

FIG. 2. (a) Feynman diagrams corresponding to the renormalized polarization operator Π, written as a sum of diagrams accounting for processes of multiple re-emissions and re-absorptions. (b) Dyson equation for the operator $\Pi(q,\omega)$. The vertices g of the bubble diagrams denote the coupling constant between the cavity photon and interband excitation and the dashed line corresponds to the bare cavity photon Green's function D_0. (c) Dyson equation for photon Green's function D, represented by a double dashed line, accounting for light-matter coupling.

It has singularity at $\hbar\omega=E_g$ which corresponds to the Van Hove singularity of the 1D density of states.

The dispersion of the elementary excitations of the coupled quantum wire-cavity system can be found from the poles of the renormalized Green's function of the cavity photon, accounting for the light-matter coupling $D(q,\omega)$. The corresponding Dyson equation is shown in diagrammatic form in Fig.2(c). Its solution reads

$$D(q,\omega)=\frac{D_0(q,\omega)}{1-g^2D_0(q,\omega)\Pi_0(q,\omega)}. \quad (15)$$

Note that $\Pi_0\sim L$ and $g\sim L^{-1/2}$, and observable quantities do not depend on the length of the system L.

III. RESULTS

We calculate the renormalized polarization operator of cavity-excitation system using Eq. (3), and find the energy spectrum of new modes. The absorption spectrum is calculated from the imaginary part of Π using Eq. (13), whilst the dispersion relations are given by its wave vector q dependence. We used standard parameters for a

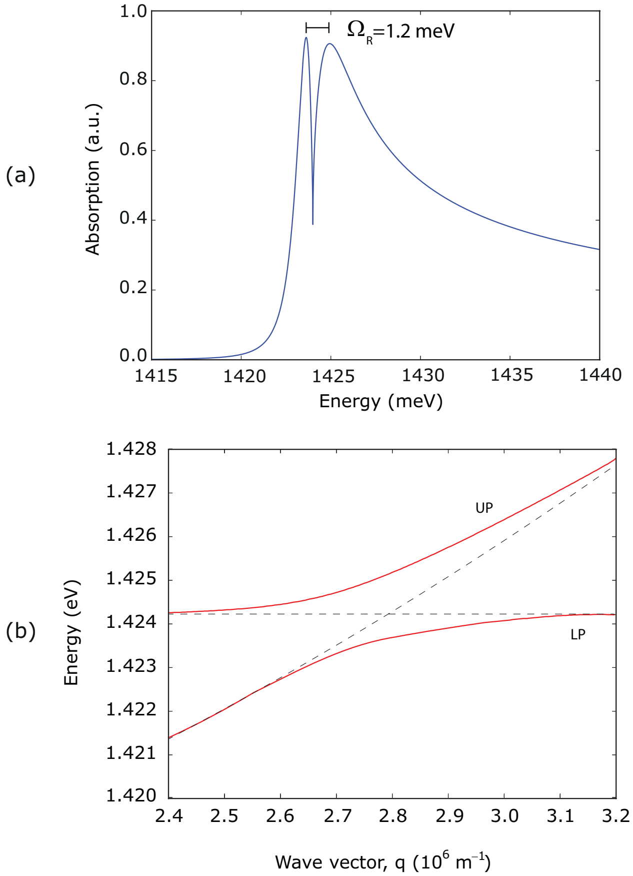

FIG. 3. (Color online) (a) An absorption plot showing polariton states formed by a microcavity photon and interband excitation in a 1D nanowire. (b) The dispersion of elementary excitations in a system. Both plots are for one quantum wire and a photon lifetime of $\tau_{ph} = 10$ ps, which corresponds to $\gamma = 0.4$ meV. These parameters yield a Rabi frequency of $\hbar\Omega_R = 1.2$ meV.

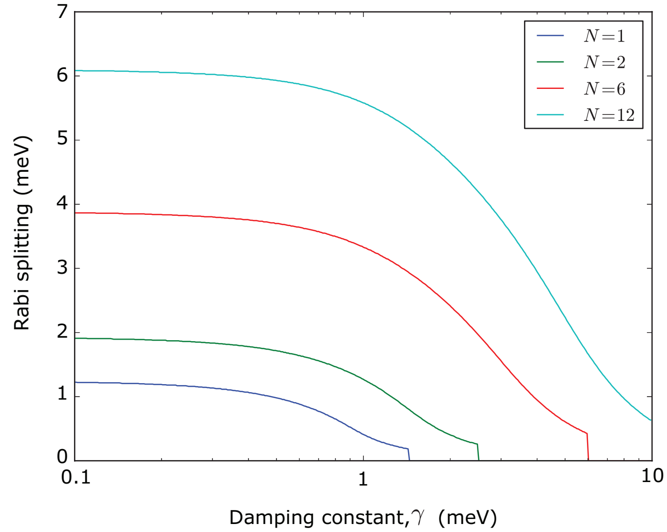

FIG. 4. (Color online) The Rabi splitting as a function of the cavity photon damping constant γ plotted for different numbers of quantum wires N embedded into a semiconductor microcavity.

GaAs sample in our calculations.

Fig. 3 shows the absorption spectrum of the coupled GaAs quantum wire-cavity system and dispersion relation of the emergent polaritonic modes. The lifetime of the cavity photon was taken as $\tau_{ph} = 10$ ps and the detuning of the cavity mode is $\delta = -10$ meV. One can clearly see the anti-crossing of the eigenmodes, characteristic for the strong coupling regime. The value of the Rabi splitting for parameters considered here is about $\hbar\Omega_R = 1.2$ meV for a single quantum wire embedded into a microcavity. The formation of polaritons is also revealed by a double peak structure of the absorption spectrum shown in Fig. 3(a).

The Rabi splitting can be enhanced by placing more than one wire in the cavity. In this case the polarization operator corresponding to a single wire Π_0 should be replaced by $N\Pi_0$, where N is the number of wires in the cavity. The decrease of the quality of the cavity, corresponding to the increase of the cavity mode broadening γ, results in quenching of the Rabi splitting. The corresponding dependence for different values of N is shown in Fig. 4. The damping constant γ scales from 0.1 to 10 meV on a logarithmic scale which corresponds to the lifetimes spanning from 40 to 0.4 ps, which are possible to realize experimentally.

One can see that for $\gamma \gtrsim 1$ meV, which corresponds to a typical quality factor of semiconductor cavities, more than one wire is required for a transition into the strong coupling regime. However, with recent improvement of nanotechnology fabrication of high quality resonators with $\gamma \sim 0.1$ meV becomes possible.[28] This in principle can allow the achievement of strong coupling for an individual wire.

Our calculations are restricted to zero temperature, $T = 0$ K; accounting for finite temperature is less straightforward. However, because of the sharp behavior of the 1D density of states, we expect that the predicted effects will be still pronounced. The possible drawbacks of broadening of the excitation mode with higher temperature, which reduces the Rabi frequency, can be possibly overcome in systems containing $N > 10$ wires embedded in a high-quality cavity with $\gamma \lesssim 1$ meV. In this situation, one might expect to achieve strong coupling for a gallium arsenide system at room temperature, similarly to the case of intersubband transitions.[20] Note, that semiconductor quantum wires can be replaced by carbon nanotubes, which are commonly synthesized in bundles[29] or can be arranged in well-aligned arrays.[30] In general, excitonic effects are very important in semiconducting carbon nanotubes, as the presence of strongly-bound dark excitons results in the luminescence suppression.[31] However, tuning the cavity mode to the nanotube's Van Hove singularity should significantly improve light-matter cou-

pling. In quasi-metallic nanotubes with small curvature-induced band gaps and in metallic (armchair) nanotubes with magnetic-field-induced gaps, excitonic effects can be neglected;[32] so that our theory of Van Hove polaritons becomes directly applicable. Narrow-gap carbon nanotubes have recently attracted significant attention as promising candidates for terahertz applications.[33–35] Metallic nanotubes with magnetic-field-induced gaps are of a particular interest, since their spectra can be easily tuned by an external magnetic field. Their similarity to a two-level system is further enhanced by the fast decrease of the dipole transition matrix element away from the field-induced bandgap.[36] Another system, for which the developed theory is highly relevant, is a bulk semiconductor with Van Hove singularities resulting from the quasi-one-dimensional motion along a quantizing magnetic field. Carbon nanotubes in microcavities in both the optical and terahertz frequency range as well as bulk materials with magnetic-field-induced Van Hove singularities are a subject of our future work.

IV. CONCLUSIONS

In conclusion, we have studied the light-matter coupling of a microcavity photon and interband transition in a 1D nanowire. Due to the resonant character of the absorption spectrum provided by the Van Hove singularity of the 1D density of states, the achievement of the strong coupling regime becomes possible even in the absence of excitonic effects. We have calculated the dispersions of resulting polariton modes and the absorption spectra of the coupled wire-cavity system for realistic values of parameters. The dependence of the Rabi frequency on the broadening of the cavity mode was investigated for different numbers of the wires embedded into cavity.

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